201-15002B

IUCLID

Data Set

Existing Chemical

CAS No.

EC No.

TSCA Name

EINECS Name

: 200-589-6 : Sulfuric acid, diethyl ester

: C4H10O4S Molecular Formula

Producer related part

Company

: The Dow Chemical Company

Creation date : 12.09.2003

Substance related part

Company

Creation date

: The Dow Chemical Company

: 12.09.2003

: ID: 64-67-5

: diethyl sulphate

: 64-67-5

Status

Memo

Printing date Revision date : 18.12.2003

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: 45

Chapter (profile) Reliability (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10

Reliability: without reliability, 1, 2, 3, 4 Flags (profile)

: Flags: without flag, confidential, non confidential, WGK (DE), TALuft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

ld 64-67-5 **Date** 18.12.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Туре

Name : SIBER HEGNER RAW MATERIALS LTD.

Contact person

Date .

Street : WIESENSTRASSE 8
Town : CH-8022 Zurich
Country : Switzerland

Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Flag : non confidential

23.10.1995

Type

Name : Union Carbide Benelux

Contact person

Date

Street: Norderlaan 147Town: 2030 Antwerpen

Country : Belgium

Phone

Telefax

Telex

Cedex Email

Homepage

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Flag : non confidential

23.10.1995

Туре

Name : Whyte Chemicals Ltd

Contact person

Date

Street : 322 Regents Park Road

Town : N3 2UA London Country : United Kingdom

Phone :

Telefax :
Telex :
Cedex :
Email :
Homepage :

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Flag : non confidential

23.10.1995

ld 64-67-5 **Date** 18.12.2003

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type

Substance type : organic
Physical status : liquid
Purity : > 99 - % w/w

Colour : Odour :

Remark : Diethyl Sulfate specification has a purity requirement of 99.5 wt %. The

product as normally produced and received into the distribution system in 2002 had an average purity of 99.78 wt %. GC analysis of the storage tank for the year 2002 showed an average purity of 99.77 wt %, with a minimum

and maximum purity of 99.65 and 99.87 wt %, respectively.

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Flag : non confidential

17.12.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Diethyl Sulphate

Source : SIBER HEGNER RAW MATERIALS LTD. Zurich

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

ethyl sulfate

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

ETHYLSULPHATE

Source : Whyte Chemicals Ltd London

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

ld 64-67-5 **Date** 18.12.2003

sulfuric acid, diethyl ester

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)
UNION CARBIDE CORPORATION Houston

23.10.1995

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Labelling : as in Directive 67/548/EEC

Specific limits: noSymbols: T, , ,Nota: E, ,

R-Phrases : (45) May cause cancer

(46) May cause heritable genetic damage

(20/21/22) Harmful by inhalation, in contact with skin and if swallowed

(34) Causes burns

S-Phrases : (53) Avoid exposure - obtain special instructions before use

(45) In case of accident or if you feel unwell, seek medical advice

immediately (show the label where possible)

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Flag : non confidential

23.10.1995

1.6.2 CLASSIFICATION

Classified : as in Directive 67/548/EEC
Class of danger : carcinogenic, category 2
R-Phrases : (45) May cause cancer

Specific limits :

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Flag : non confidential

23.10.1995

Classified : as in Directive 67/548/EEC

Class of danger : corrosive

R-Phrases : (34) Causes burns

Specific limits :

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

ld 64-67-5 **Date** 18.12.2003

Flag : non confidential

23.10.1995

Classified : as in Directive 67/548/EEC

Class of danger : harmful

R-Phrases : (20/21/22) Harmful by inhalation, in contact with skin and if swallowed

Specific limits :

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Flag : non confidential

23.10.1995

Classified : as in Directive 67/548/EEC Class of danger : mutagenic, category 2

R-Phrases : (46) May cause heritable genetic damage

Specific limits

Source : ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Flag : non confidential

23.10.1995

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : MAK (DE) **Limit value** : .03 ml/m3

Source : SIBER HEGNER RAW MATERIALS LTD. Zurich

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

Type of limit : TLV (US)

Limit value

Remark : 1 ppm-skin: TLV-TWA

Union Carbide recommendation

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

ld 64-67-5 **Date** 18.12.2003

UNION CARBIDE CORPORATION Houston

23.10.1995

Remark : 1 PPM - SKIN TWA

Source : Whyte Chemicals Ltd London

ECB - Existing Chemicals Ispra (VA)
UNION CARBIDE CORPORATION Houston

23.10.1995

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark: As the quantities of this substance placed on the EU market

by Union Carbide Benelux N.V. are normally sourced from the manufacturing facilities of its U.S. parent company, no exposure can arise within the EU from the manufacture of these quantities. The comments below on exposure are restricted to uses for which Union Carbide believes its

customers use this substance.

Major use(s): chemical intermediate for dyes, pharmaceuticals etc. always used in closed systems.

Sources of human exposure: negligible assuming appropriate industrial hygiene and personal protection precautions are observed. There are no consumer uses, hence no public exposure.

Sources of environmental exposure: none - this substance is chemically transformed into other substances. Releases to waste water systems hydrolyse to ethanol (inherently

biodegradable) and sulphuric acid.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

ld 64-67-5 **Date** 18.12.2003

UNION CARBIDE CORPORATION Houston

23.10.1995

Remark: Diethyl Sulfate is used for basic organic synthesis. When

handling according to the basic precaution rules (avoid all possible contact with the product) no harm whether to humans nor to the environemt are to be expected.

Source : SIBER HEGNER RAW MATERIALS LTD. Zurich

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

16.09.2003

Country : Germany MAK-LIST: Group IIIA2

Source : SIBER HEGNER RAW MATERIALS LTD. Zurich

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

Remark : DES IS PRODUCED IN A CLOSED PROCESS. THE ONLY POSSIBLE

EXPOSURE TO HUMANS AND ENVIRONMENT IS VIA AN

ACCIDENTIAL

RELEASE. NO FURTHER INFORMATION AVAILABLE.

Source : Whyte Chemicals Ltd London

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

16.09.2003

1.11 ADDITIONAL REMARKS

Remark : Disposal: Incinerate in a furnace where permitted under

appropriate national and local regulations. May be mixed with solvent (acetone) for ease in burning. In very dilute concentrations (about 10 ppm) in water, it may be amenable to biodegradation in a treatment plant, but the acidity resulting from hydrolysis must be carefully monitored and

neutralized.

Transport: Diethyl sulphate is classified as class 6.1 product according the ADR/RID/IMDG/ICAO regulations. Diethyl sulphate is shipped in appropriate road and rail transport units and smaller packages (e;g. drums). The product has to be loaded, unloaded or transloaded with a vapour return line. Every container used for diethyl

sulphate shall have no bottom outlets. Only top-loading and

unloading is allowed.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

16.09.2003

Remark : NO ADDITIONAL REMARKS.
Source : Whyte Chemicals Ltd London

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

ld 64-67-5 **Date** 18.12.2003

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

ld 64-67-5 **Date** 18.12.2003

2.1 MELTING POINT

Value : $= -24.5 - {}^{\circ}\text{C}$

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

03.11.2003 (6)

Value : -25 - °C

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (28)

Value : -24.4 - °C

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (22) (38)

2.2 BOILING POINT

Value : $= 208 - ^{\circ}C$ at

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

03.11.2003 (6)

Value : 208 - °C at

Decomposition : yes Method : Year :

GLP :

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (22)

Value : 209.5 - °C at

Decomposition : yes

Method : Year : GLP :

Test substance

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (28)

Decomposition : yes Method : Year :

ld 64-67-5 **Date** 18.12.2003

GLP :

Remark: decomposes to ethyl ether, ethylene and sulphur oxides at

temperatures above 100 degrees C.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (38)

2.3 DENSITY

Type : density

Value : = $1.1774 - \text{g/cm}^3 \text{ at } 20 \text{ °C}$

Reliability : (2) valid with restrictions

03.11.2003 (6)

Type : relative density
Value : 1.1795 - at 20 °C

Method

Year :

GLP : no data

Test substance

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (38)

Type : relative density
Value : 1.172 - at 28 °C

Method

Year

GLP : no data

Test substance

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (28)

Type : density

Value : 1.1803 - at °C

Method

Year

GLP : no data

Test substance :

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (22)

2.3.1 GRANULOMETRY

ld 64-67-5 **Date** 18.12.2003

2.4 VAPOUR PRESSURE

Value : = .19078 - hPa at 20 °C

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

03.11.2003 (27)

Value : .13 - hPa at 20 °C

Decomposition : Method :

Year

GLP : no data

Test substance

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (38)

Value : .25 - hPa at 20 °C

Decomposition

Method Year

GLP : no data

Test substance

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (22)

Value : 1.33 - hPa at 47 °C

Decomposition

Method

Year : GLP :

Test substance :

Source : Union Carbide Benelux Antwerpen

no data

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (28)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water Log pow : = 1.14 - at °C

pH value :

Method : other (calculated): EPIWIN (v 3.11) KOWWIN Submodel (v 1.67)

Year : 2003

GLP : Test substance :

Remark: The EPIWIN model was run using the following measured physical

chemical properties:

Vapor pressure (mm Hg): 0.14344; Boiling point (deg C): 208.0; and Melting point (deg C): -24.50.

ld 64-67-5 **Date** 18.12.2003

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

15.12.2003 (31)

Partition coefficient

Log pow : 1.14 - at °C

pH value : Method :

Year

GLP : no data

Test substance: as prescribed by 1.1 - 1.4

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

07.11.2003 (37)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water

Value : = 7000 - mg/l at 20 °C

pH value : -

concentration : at °C

Temperature effects

Examine different pol.

pKa : at 25 °C

Description :

Stable

Reliability : (2) valid with restrictions

:

:

:

Flag : Critical study for SIDS endpoint

25.11.2003 (15)

Solubility in : Water

Value : - at °C

pH value : -

concentration : at °C

Temperature effects

Examine different pol.

pKa : at 25 °C

Description :

Stable

Remark: Insoluble, decomposes at room temperature.

Reliability : (2) valid with restrictions

25.11.2003 (6)

Remark : 0.7% by weight solubility in water at 20 degrees C. Diethyl

sulphate reacts vigorously with water.

Source : Union Carbide Benelux Antwerpen ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

09.10.2003 (38)

Remark: Practically insoluble in water and gradually decomposed by

it. Rapidly decomposition by hot water into monoethyl

sulfate and alcohol.

Source : Union Carbide Benelux Antwerpen

ld 64-67-5 **Date** 18.12.2003

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (28)

Remark: Insoluble in water.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (22)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : 104 °C Type : closed cup

Method : other: Tag Closed Cup (ASTM D 56)

Year

GLP : no data

Test substance

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (22) (28) (38)

2.8 AUTO FLAMMABILITY

Value : 436 - °C at

Method

Year

GLP : no data

Test substance :

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (22)

2.9 FLAMMABILITY

Result : other: no data to report

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

2.10 EXPLOSIVE PROPERTIES

Remark: Flammability limits in air (% by weight):

- lower: 4.1

Id 64-67-5 Date 18.12.2003

- upper: not determined

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (39)

2.11 OXIDIZING PROPERTIES

Result : other: no data to report

Source Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

Remark : vapour density (air = 1): 5.3

Source : Union Carbide Benelux Antwerpen ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (38)

ld 64-67-5 **Date** 18.12.2003

3.1.1 PHOTODEGRADATION

DIRECT PHOTOLYSIS

Halflife t1/2 : = 6.5 - day(s)**Degradation** : - % after

Quantum yield Deg. product

Method : other (calculated): EPIWIN (v 3.11) AOP Submodel (v 1.91)

Year : 2003

GLP :

Test substance :

Remark : Overall OH rate constant = 1.6422 E-12 cm3/molecule/sec

The EPIWIN model was run using the following measured physical

chemical properties:

Vapor pressure (mm Hg): 0.14344; Boiling point (deg C): 208.0; and Melting point (deg C): -24.50.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

15.12.2003 (29)

Remark : Nihil

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

06.10.2003

3.1.2 STABILITY IN WATER

Remark: Decomposes gradually to alcohol and sulfuric acid.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

Deg. products : 64-17-5 Ethanol

7664-93-9 Sulfuric acid

12.11.2003 (6)

3.1.3 STABILITY IN SOIL

Remark: Decomposes gradually by reaction with moisture in soil to

alcohol and sulfuric acid

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

ld 64-67-5 **Date** 18.12.2003

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : other: air (emissions to compartment = 1000 kg/hr)

Method : Calculation according Mackay, Level III

Year : 2003

Method : Equilibrium Concentration Model (EQC) Level III

Remark : The EPIWIN model was run using the following measured physical

chemical properties:

Vapor pressure (mm Hg): 0.14344; Boiling point (deg C): 208.0; and Melting point (deg C): -24.50.

Result : Concentration (%):

Air - 77 Water - 15 Soil - 9 Sediment - < 0.1

Level III Fugacity Model (Full-Output):

Chem Name : Sulfuric acid, diethyl ester

Molecular Wt: 154.18

Henry's LC: 8.4e-006 atm-m3/mole (Henry database)

Vapor Press: 0.143 mm Hg (user-entered) Log Kow : 1.14 (Kowwin program) Soil Koc : 5.66 (calc by model)

Mass Amount Half-Life Emissions (percent) (hr) (kg/hr) Air 1000 76.6 143 Water 14.7 360 0 Soil 8.7 360 0 1.44e+003 0 Sediment 0.0274

Reaction Advection Reaction Advection Fugacity (percent) (percent) (atm) (kg/hr) (kg/hr) Air 63.9 1.01e-010 311 639 31.1 Water 3.34e-012 23.6 12.3 2.36 1.23 5.04e-011 14 Soil 0 1.4 0

Sediment 2.74e-012 0.011 0.000458 0.0011 4.58e-005

Persistence Time: 83.5 hr Reaction Time: 240 hr Advection Time: 128 hr Percent Reacted: 34.8 Percent Advected: 65.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 142.6 Water: 360

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Soil: 360 Sediment: 1440

Biowin estimate: 2.858 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

15.12.2003 (32)

Media : other: water (emissions to compartment = 1000 kg/hr)

Method : Calculation according Mackay, Level III

Year : 2003

Method : Equilibrium Concentration Model (EQC) Level III

Remark : The EPIWIN model was run using the following measured physical

chemical properties:

Vapor pressure (mm Hg): 0.14344; Boiling point (deg C): 208.0; and Melting point (deg C): -24.50.

Result : Concentration (%):

Air - < 1 Water - 99 Soil - < 0.1 Sediment - < 1

Level III Fugacity Model (Full-Output):

Chem Name : Sulfuric acid, diethyl ester

Molecular Wt: 154.18

Henry's LC: 8.4e-006 atm-m3/mole (Henry database)

Vapor Press: 0.143 mm Hg (user-entered) Log Kow : 1.14 (Kowwin program) Soil Koc : 5.66 (calc by model)

Mass Amount		Half-Life	Emissions
	(percent)	(hr)	(kg/hr)
Air	0.527	143	0
Water	99.2	360	1000
Soil	0.0598	360	0
Sediment 0.185		1.44e+0	03 0

Fugacity Reaction Advection Reaction Advection (atm) (kg/hr) (kg/hr) (percent) (percent) Air 2.8e-012 8.58 17.7 0.858 1.77 Water 9.06e-011 640 333 64 33.3 Soil 1.39e-012 0.386 0 0.0386 0 Sediment 7.44e-011 0.298 0.0124 0.0298 0.00124

Persistence Time: 335 hr Reaction Time: 516 hr Advection Time: 957 hr Percent Reacted: 65 Percent Advected: 35

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 142.6 Water: 360 Soil: 360 Sediment: 1440

ld 64-67-5 **Date** 18.12.2003

Biowin estimate: 2.858 (weeks)

Advection Times (hr):
Air: 100
Water: 1000

Sediment: 5e+004
(2) valid with restrictions

Flag : Critical study for SIDS endpoint

15.12.2003 (32)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Reliability

Type : aerobic

Inoculum : other: microbial seed

Contact time

Degradation : $57 - (\pm) \%$ after 20 day(s)

Result :

Kinetic of testsubst. : 5 day(s) 25- %

10 day(s) 30 - % 20 day(s) 57 - %

- % - %

Deg. product

Method : other: BOD20

Year : 1974 GLP : no Test substance :

Remark : The test method utilized was: "Standard Methods for the Examination of

Water and Wastewater." 1971. 13th edition, Amer. Pub. Health Assn., New York, NY. A settled domestic wastewater was filtered through glass wool and then added (3 ml/bottle) as seed material to clean 300 ml BOD bottles. The dilution water was sparged with pure oxygen to produce an available DO level of 30 to 35 mg/l and added to the seed material to completely fill the bottles. The pure chemical was added to each bottle (3.0 µl/bottle) to provide a concentration of approximately 10 mg/l. At least two of the concentrations were tested in duplicate. Dissolved oxygen content was measured approximately five times throughout the test using a commercial DO meter filled with an agitated probe. When the DO level dropped below 4.0 mg/l, the contents were reaerated. Samples (2 ml) were analyzed routinely for nitrites and nitrates throughout the study because ammonia nitrogen and organic nitrogen contained in the test system could be oxidized to form these two compounds. No attempt was made to inhibit nitrification. Appropriately seeded blanks and glucose standards were prepared during each test run using the same dilution water used for the test samples.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

13.11.2003 (20) (40)

3.6 BOD5, COD OR BOD5/COD RATIO

ld 64-67-5 **Date** 18.12.2003

COD

Method : other

Year

COD : 1.25 mg/g substance

GLP

Remark: calculated THOD

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

3.7 BIOACCUMULATION

Remark: Based on the estimated Log Kow of 1.14 and the rapid hydrolysis of DES in

water, the bioaccumulation potential is considered to be very low.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

17.12.2003

3.8 ADDITIONAL REMARKS

4. Ecotoxicity ld 64-67-5

Date 18.12.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Туре

Species: Pimephales promelas (Fish, fresh water)

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : 95

Limit test :

Analytical monitoring : no data

Remark : test references:

(1) Methods for Measuring the Acute Toxicity of Effluents

to Freshwater and Marine Organisms, EPA/600/4-85/013, March

1985.

(2) Annual Book of ASTM standards, Water and Environmental

Technology, Vol. 111.04, (1990). Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

09.12.2003 (41)

Туре

Source

Species : Salmo gairdneri (Fish, estuary, fresh water)

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : 20

Limit test

Analytical monitoring: no dataMethod: otherYear: 1988GLP: no dataTest substance: no data

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (18)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Туре

Species : Daphnia sp. (Crustacea)

Exposure period : 48 hour(s)
Unit : mg/l

EC50 : = 742.393 - calculated

Method: other: EPIWIN (v 3.11) ECOSAR Submodel (v 0.99g)

Year : 2003

GLP :

Test substance :

Remark: The EPIWIN model was run using the following measured physical

chemical properties:

Vapor pressure (mm Hg): 0.14344; Boiling point (deg C): 208.0; and Melting point (deg C): -24.50.

15.12.2003 (30)

4. Ecotoxicity ld 64-67-5

Date 18.12.2003

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae:Green algae

Endpoint

Exposure period : 96 hour(s)
Unit : mg/l

EC50 : = 5.192 - calculated

Method : other: EPIWIN (v 3.11) ECOSAR Submodel (v 0.99g)

Year : 2003

GLP : Test substance :

Remark : The EPIWIN model was run using the following measured physical

chemical properties:

Vapor pressure (mm Hg): 0.14344; Boiling point (deg C): 208.0; and Melting point (deg C): -24.50.

15.12.2003 (30)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

ld 64-67-5 5. Toxicity Date 18.12.2003

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

LD50 Type

880 - mg/kg bw Value

Species rat

Strain

Sex

Number of animals

Vehicle

Doses

Method other: acute oral toxicity :

:

:

Year 1949 : **GLP** : nο

Test substance as prescribed by 1.1 - 1.4

Remark Rat strain was Wistar or Sherman. Six animals per dose group were dosed

with the test substance.

LD50 value is calculated using the method of Thompson, W. R. (1947. Use of moving averages and interpolation to estimate median-effective

dose. Bact. Reviews, 11:115)

Result 95% confidence limits: 760-1010 mg/kg. Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Test substance : Test substance administered as a 10% solution in corn oil.

Reliability (2) valid with restrictions

Critical study for SIDS endpoint Flag

04.11.2003 (24)

5.1.2 ACUTE INHALATION TOXICITY

Type LC50

Value 250 - 500 ppm

Species rat Strain

Sex

Number of animals 12

Vehicle Doses

Exposure time

4 hour(s) Method other Year 1949 **GLP** : no

Test substance as prescribed by 1.1 - 1.4

Remark 0/6 killed at 250 ppm; 6/6 killed at 500 ppm Source Union Carbide Benelux Antwerpen ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Reliability (2) valid with restrictions Flag : Critical study for SIDS endpoint

17.12.2003 (24)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50

Value : 706 - mg/kg bw

Species : rabbit

Strain :

Number of animals
Vehicle
Doses

Method : other: acute dermal toxicity

Year : 1951 **GLP** : no

Test substance: as prescribed by 1.1 - 1.4

Remark : Original data reported as 600 ml/kg; 95% confidence for

value = 430-840 ml/kg; LD50 calculated based on density of 1.1774 g/ml.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

03.11.2003 (35)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : LD50

Value : 350 - mg/kg bw

Species : rat

Strain

Sex

Number of animals

Vehicle

Doses

Route of admin.

Exposure time :

Method : no data

Year

GLP : no data
Test substance : no data

Source : Union Carbide Benelux Antwerpen

S.C.

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

01.10.2003 (42)

5.2.1 SKIN IRRITATION

Species : rabbit

Concentration : Exposure : Exposure time : 5
Vehicle : PDII : 5

Result : irritating

Classification

Method : Draize Test

Year : 1949 **GLP** : no

Test substance: as prescribed by 1.1 - 1.4

Remark : Application: 11mg (0.01 ml) applied to the clipped abdomen - the

application site remained uncovered and was observed 24 hr after

application.

Result : necrosis observed

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

04.11.2003 (24)

Species : rabbit
Concentration : undiluted

Exposure

Exposure time : 4 hour(s)

Number of animals : 6 Vehicle :

PDII

Result : irritating

Classification

Method : other: USDOT Skin Irritancy Test (Modified)

Year : 1982 GLP : no data

Test substance: as prescribed by 1.1 - 1.4

Remark: Application period: 4hr, 589 mg (0.5ml, undiluted test substance) covered.

Both the skin and the gauze patch were moistened with saline before the test substance was applied. Skin reactions were recorded according to the

system of Draize at one hour, one day and two days after application.

Result : 4/6 with ecchymosis and slight to severe edema,

2/6 with erythema and slight to severe edema,

none had necrosis.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)
UNION CARBIDE CORPORATION Houston

Conclusion : not corrosive

04.11.2003 (33)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted

Dose : Exposure time : Comment : Number of animals : 1

Result : irritating

Classification : risk of serious damage to eyes

Method : other Year : 1949 GLP : no

Test substance: as prescribed by 1.1 - 1.4

Remark: Method: see Carpenter, C.P. and Smyth, H.F. (1946),

Am.J.Ophtal. 29:1363-1372; and Smyth,H.F. and Carpenter,C.P.(1944), J.Ind.Hyg.Toxicol. 26:269-273. Volumes installed: 0.001, 0.005, 0.02ml (1.18, 5.9,

23.6 mg) applied directly to the cornea.

Result: Severe corneal injury.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

04.11.2003 (24)

5.3 SENSITIZATION

Remark: No information available.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)
UNION CARBIDE CORPORATION Houston

23.10.1995

5.4 REPEATED DOSE TOXICITY

Remark: See section 5.7

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)
UNION CARBIDE CORPORATION Houston

23.10.1995

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Salmonella typhimurium reverse mutation assay

System of testing : TA100

Test concentration : 500, 1000, 2000, and 4000 ug/plate

Cycotoxic concentr. : None
Metabolic activation : without
Result : positive
Method : other
Year : 1992
GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Method: This assay was carried out with S. typhimurium TA100 in the absence of

S9 mixture using the preincubation method (Maron, D.M. and B.N. Ames. 1983. Revised methods for the Salmonella mutagenicity test, Mutation Res., 113:173-215). The reaction mixture consisted of 0.5 ml of phosphate buffer, 0.1 ml of a solution of the test substance prepared at gradient concentration, and 0.1 ml of the cell suspension grown for 8 h at 37 C. Dose concentrations ranged from 500 to 4000 μ g/plate. Duplicate plates were run at each dose level for the test substance and solvent controls. A confirmatory assay also was conducted. The test was considered positive when the number of revertant colonies (mean value of two plates) was more than twice that of the solvent control in a dose-dependant manner and the reproducibility of the results was confirmed by a second assay.

Result: In this study, the mutagenicity of diethyl sulfate was

demonstrated using a preincubation reverse assay in S. typhimurium TA100 without any metabolic activation. The results of the test showed a dose-dependent increase in the number of revertant colonies that was more than twice the

solvent control.

Dose (µg/plate) His+ revertants/plate

 $\begin{array}{lll} 0 \text{ (solvent control)} & 136 \pm 5 \\ 500 & 138 \pm 4 \\ 1000 & 834 \pm 1 \\ 2000 & 4801 \pm 48 \\ 4000 & 4261 \pm 81 \end{array}$

Note: results are the mean \pm SD of counts from duplicate plates.

Source : UNION CARBIDE CORPORATION Houston

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

17.11.2003 (19)

Type : HGPRT assay

System of testing : Chinese Hamster Ovary (CHO) cells

Test concentration: 0.08% by volume without S9 activation, 0.04% by volume with S9

activation

Cycotoxic concentr.

Metabolic activation: with and without

Result : positive
Method : other
Year : 1980
GLP : no

Test substance: as prescribed by 1.1 - 1.4

Method

CHO cells were exposed for 5 hours to five concentrations of diethyl sulfate from 0.08% (by volume) without the addition of an S9 metabolic activation system and from 0.04% to 0.0025% with S9 activation. In a second, repeat test identical concentrations were tested with S9, and one additional, lower concentration (0.0025%) was tested without S9 activation. Dilutions of diethyl sulfate for testing were prepared by either direct addition of the test agent into the cell culture media or by making sequential one-half dilutions in glass distilled DMSO. The surviving fraction was determined at 20 to 24 hours after treatment and the mutant fraction was determined after a 7 to 10 day period to allow "expression" of the mutant phenotype. S9 liver homogenate was prepared from Aroclor 1254-induced Sprague-Dawley male rats. Appropriate dose levels of positive, negative (deionized water) and solvent (DMSO) controls were used.

Result

: An apparent dose response effect upon cytotoxicity was observed for the concentrations of test substance tested with or without S9 activation in comparison to the values for the solvent or negative controls; although a slight difference in cytotoxicity was seen in the two experiments. The following table provides the percent survival data for the two independent experiments:

1	Experi	ment 1	Experir	ment 2		
Concentration	% Sı	urvival	% Su	% Survival		
(%, v/v)	-S9	+S9	-S9	+S9		
0.080	0	(NT)	0	(NT)		
0.040	3.0	0.1	14.0	2.1		
0.020	18.8	3.0	34.0	39.2		
0.010	31.2	11.0	51.5	45.5		
0.005	36.0	24.2	55.5	57.5		
0.0025	(NT)	31.0	53.2	51.0		
DMSO control	45.5	43.8	52.5	47.8		
Neg. control	47.8	35.0	37.0	67.0		
(NT) = Not Tested						

Significant increases in the mutant frequency were obtained which indicated a dose-related induction of the frequency of mutants/10⁶ viable cells over the 16-fold range of concentrations tested for potential mutagenic action either

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> with or without the presence of an S9 metabolic activation system. All tested concentrations of diethyl sulfate produced an increase in the mutation frequency which was statistically significant from the concurrent solvent control in the test either with or without S9 activation. These significant mutagenicity data were considered to be a biologically significant indication of a positive effect. The data also indicated the presence of a dose-related increase in the number of mutants induced by treatment which is considered an important criterion of a positive mutagenic response. Diethyl sulfate was considered to be a mutagenic agent based upon the data. The following table provides the mutant frequency results with and without S9 activation:

Experim	nent 1	Experim	ent 2		
n Mutai	nts (a)	Mutar	Mutants (a)		
-S9	+S9	-S9	+S9		
382.2*	(NT)	TOXIC	(NT)		
1385.9*	663.3*	811.1*	1267.3*		
672.9*	951.2*	1021.8*	770.7*		
525.3*	472.7*	432.7*	699.0*		
332.7*	131.2*	303.4*	598.0*		
(NT)	289.2*	198.4	273.7*		
l 88.6	50.7	123.4	35.5		
170.3*	73.9	18.7	57.5		
	Mutar -S9 382.2* 1385.9* 672.9* 525.3* 332.7* (NT)	-S9 +S9 382.2* (NT) 1385.9* 663.3* 672.9* 951.2* 525.3* 472.7* 332.7* 131.2* (NT) 289.2* I 88.6 50.7	Mutants (a) Mutants (a) -S9 +S9 -S9 382.2* (NT) TOXIC 1385.9* 663.3* 811.1* 672.9* 951.2* 1021.8* 525.3* 472.7* 432.7* 332.7* 131.2* 303.4* (NT) 289.2* 198.4 I 88.6 50.7 123.4		

(a) = Total # mutant colonies per 10^6 cells plated divided by viable fraction.

Source UNION CARBIDE CORPORATION Houston

11.11.2003 (36)

Sister chromatid exchange assay Type System of testing Chinese Hamster Ovary (CHO) cells

Test concentration : 0.02% to 0.00125%

Cycotoxic concentr. : 0.02% Metabolic activation without positive Result Method other 1980 Year GLP

Test substance as prescribed by 1.1 - 1.4

Method

Dilutions of diethyl sulfate for testing, ranging from 0.02% to 0.00125% (by volume), were prepared either by direct addition into the culture medium or by making sequential one-half dilutions of the maximum dose level in DMSO. For determination of direct mutagenic action, CHO cells were exposed to diethyl sulfate and appropriate controls for 5 hours without S9 activation. Indirect mutagenic action requiring metabolic activation by liver S9 homogenate, was not studied because of the highly significant positive responses observed in the experiment without S9. Chemicals which produce a highly significant response by direct action are considered mutagenic regardless of the response obtained

with S9. BrdU required to differentiate between the

individual "sister" chromatids by SCE staining, was present at a concentration of 3 ug/mL in the growth medium during treatment and during the culture period following exposure.

A total of 15 cells/dose level and 5 dose levels,

without metabolic activation were examined. Appropriate dose levels of positive, negative (deionized water) and solvent (DMSO) controls were used. Ethylmethanesulfonate was used as the positive control substance

^{*} Significantly different from DMSO control (p<0.05, Student's t-test)

Result

without metabolic activation.

A statistically-significant increase in the SCE frequency was produced by two of the dose-levels of diethyl sulfate tested for direct action in the absence of a metabolic activation system. The test without S9 activation was considered a positive indication of potential direct mutagenic action of diethyl sulfate. An increase in the frequency of SCE corresponding to increased dose-levels of diethyl sulfate was readily apparent from 0.00125% to 0.01% which indicated a probable biological significance of these results. The 0.02% concentration was cytotoxic and inhibited the appearance of cells with SCE staining, possibly because of effects of the test agent on cell growth. The sample of diethyl sulfate was classified as a positive mutagenic agent by direct action and testing with an S9 activation system was not performed. Treatments of CHO cells with diethyl sulfate over a 16-fold range of concentrations indicated a significant potential for mutagenic activity in tests of direct mutagenic action without addition of an active S9, metabolic activation system. Evidence of a dose-related effect of diethyl sulfate exposure on the SCE frequency was evident and the test agent was considered to be an active agent in the in vitro assay. Following is a table of results:

Concentration Mean number of SCE/chromosome

(%, v/v) (+/- S.D.)
0.020 0.474 (0.130) @
0.010 2.192 (0.825)*
0.005 1.634 (0.478)*
0.0025 1.032 (0.277)
0.00125 0.868 (0.287)

DMSO control 0.871 (0.304)
Negative control 0.668 (0.125)

@ = Toxic, only 9 analyzable cells found

* = Significantly different from DMSO control (p<0.05, Student's t-test).

Source : UNION CARBIDE CORPORATION Houston

Reliability : (1) valid without restriction

11.11.2003 (36)

Type : Unscheduled DNA synthesis

System of testing : rat hepatocyte cells

Test concentration : 100 x 10^-3% to 0.1 x 10^-3% by volume

Cycotoxic concentr.

Metabolic activation: no dataResult: positiveMethod: otherYear: 1980GLP: no

Test substance: as prescribed by 1.1 - 1.4

Method: Induction of DNA damage in rat liver cells (hepatocytes),

resulting in stimulation of Unscheduled DNA Synthesis (UDS), was studied at a minimum of six dose levels which spanned a 1000-fold range of concentrations from 0.0001, 0.001, 0.003, 0.01, 0.03, and 0.1% (v/v). Cells were treated with diethyl

sulfate for 2 hours in culture medium containing 3H-thymidine, hyroxyurea and appropriate dilutions of

diethyl sulfate prepared in DMSO. Determination of UDS activity was performed by analyses of radioactive incorporation into isolated

hepatocytes nuclei or in DNA. Appropriate dose levels of positive, negative

(deionized water) and solvent (DMSO) controls were used.

Result : Diethyl sulfate stimulated a significant amount of

incorporation of radioactive thymidine in cells treated over a 1000-fold range of all test concentrations. Measurements of radioactive incorporation into either nuclei or DNA isolated and precipitated from aliquots of nuclei from the same populations of treated cells verified the activity of the positive control agents and the significant activity of the diethyl sulfate test sample. Diethyl sulfate was considered an active mutagenic agent in the test with hepatocytes.

Radioactivity
% v/v Concentration % of solvent control
0.1 193

0.1 193 0.03 312 0.01 260 0.003 281 0.001 191 0.0001 321

Source : UNION CARBIDE CORPORATION Houston

Reliability : (1) valid without restriction

13.11.2003 (36)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Micronucleus assay

Species: mouseSex: maleStrain: other: ddYRoute of admin.: i.p.Exposure period: one day

Doses : 100, 200, 400 mg/kg bw

Result : positive
Method : other
Year : 1992
GLP : no data

Test substance: as prescribed by 1.1 - 1.4

Method: 7 week old male ddY mice were used after 1 week

acclimatization. They were given commercial food pellets and water ad libitum. The doses administered were decided by referring to published LD50s but in some cases by a preliminary dose-finding experiment. Three doses of the test substance were tested with 4 mice per group, by a single intraperitoneal injection, at 100, 200, and 400 mg/kg

bw. Peripheral blood (5 μ I) was collected from a tail blood vessel. One thousand well-stained reticulocytes/animal were examined. The data at 48 hours were analyzed with Fisher's exact test to test the significance of the frequency of micronucleated reticulocytes (MNRET) at each test dose compared with the control data, which was the total MNRETs of 12 mice at

0 hours (before treatment). The significance level was 0.01.

Result: MNRET induction was observed only at the highest dose of DES (400 mg/kg bw). The following table summarizes the results:

Single dose (mg/kg) 0 24 48 72 0 0.13 ± 0.06

100 0.10 \pm 0.00 0.20 \pm 0.14 0.25 \pm 0.17 0.13 \pm 0.05 200 0.13 \pm 0.05 0.25 \pm 0.13 0.28 \pm 0.17 0.18 \pm 0.10 400 0.15 \pm 0.10 0.28 \pm 0.06 0.50 \pm 0.10* 0.17 \pm 0.06

(a) Values represent mean MNRET induction of four mice per dose group ±

SD.

* Significantly different from 0 hour, p < 0.01. UNION CARBIDE CORPORATION Houston

Source : UNION CARBIDE CORPORATION He
Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint 14.11.2003

14.11.2003 (1)

Type : Micronucleus assay

Species: mouseSex: male/femaleStrain: other: MS/Ae

Route of admin. : i.p. Exposure period : 2 days

Doses : 80 and 160 mg/kg

Result : positive
Method : other
Year : 1995
GLP : no data

Test substance: as prescribed by 1.1 - 1.4

Method : The test substance was administered by i.p. injection in olive oil. Diethyl

sulfate was given twice, 24 h apart, to MS/AE mice at 10 ml/kg. Peripheral blood was collected at time 0 (before treatment) and at 6 h intervals, 24

after the second treatment.

Result : Dose at MN/1000 RET's

				.,	•••			
a time	Sampling	# of	á	asse	esse	ed p	oer	Group Mean
(mg/kg)	time (h)	animal	S	а	ınin	nal		± SD (%)
DS (160)	0	5	2	3	2	4	4	3.0 ± 1.0
	24	4	5	9	9	12		8.8 ± 2.9
	30	4	15	20	15	12		15.5 ± 3.3
	36	4	14	13	10	16		13.3 ± 2.5
	42	4	11	12	8	8		9.8 ± 2.1
	48	4	12	7	7	9		8.8 ± 2.4
	54	4	7	8	7	5		6.8 ± 1.3
	60	4	2	2	5	2		2.8 ± 1.5
DS (80)	0	5	3	3	2	6	2	3.2 ± 1.6
	24	5	11	7	9	7	9	8.6 ± 1.7
	30	5	18	8	6	7	6	9.0 ± 5.1
	36	5	10	6	7	5	9	7.4 ± 2.1
	42	5	8	6	4	3	7	5.6 ± 2.1
	48	5	6	2	1	3	2	2.8 ± 1.9
	54	5	2	6	3	0	0	2.2 ± 2.5
	60	5	5	3	0	1	2	2.2 ± 1.9

The test substance showed peak MNRET (immature erythrocyte

with a micronucleus) responses at 30 hours.

Source : UNION CARBIDE CORPORATION Houston

14.11.2003 (7)

Type : Dominant lethal assay

Species : mouse Sex : male

Strain : other: 101/E1 x C3H/E1

Route of admin. : i.p.

Exposure period : single injection

Doses : 0, 100, 200, 300 mg/kg

Result

Method : other: rodent Dominant lethal test

Year : 1988 GLP : no data Test substance : no data

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Remark 25 mice/group; animals 80-98 days old at time of treatment

> and initial mating. Males were caged with individual F1 hybrid females for 4 day intervals for 48 days for a total

of 12 mating intervals. intraperitoneal injection

Result Positive; significantly increased pre- and

> post-implantation loss observed in the 200 mg/kg and 300 mg/kg groups. There was a non-significant increase in

pre-implantation loss for the 100 mg/kg group.

Source Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

11.11.2003 (5)

Dominant lethal assay Type

Species mouse Sex male Strain C57BL

Route of admin. other: intrascrotal injection

Exposure period single injection **Doses** 0, 6.0, 30, 150 mg/kg

Result

Method other: rodent dominant lethal test

Year 1971 **GLP** no data **Test substance** no data

Remark

- 15 male mice/group (Strain: C57BL/B6); animals 2.5-3.0 months of age. Test substance administered in physiological saline solution. Each male mated with three virgin CBA females immediately after injection; females replaced each week for six weeks. At the sixth week, three to four females were used for the mating. CBA females were killed on days 14-17 of gestation and examined for embryonic lethality. The number of live embryos (A), dead embryos (B) and the number of corpora lutea (C) were counted. The following indices were calculated:
 - 1) death rate before implantation = C (A+B)/C
 - 2) death rate after implantation = B/A+B
 - 3) survival = A/C.

The relative indices were calculated by dividing the indices of the experimental group by the corresponding index in the control group. The significance of the differences between the experimental and control indices was determined by the chi square method.

Positive at doses of 6.0 and 150 mg/kg. Result

The following table summarizes the indices relative to the control values:

			Relative Letha	ality (%)	Relative
Dose		Fertile	Before	After	Survival
mg/kg	Week	Females (%)	Implantation	n Implanta	ation Rate (%)
150	1	31	171.1*	100.0	90.5
	2	67	170.0*	131.3	84.2*
	3	88	138.4	214.0*	86.2
	4	100	132.4	151.4	91.5
	5	118	107.1	153.9	93.5
	6	89	95.1	82.0	102.3
30	1	87	97.4	143.4	96.8
	2	92	109.4	113.7	96.7
	3	118	65.3	140.4	104.5
	4	125	94.3	135.7	98.2
	5	130	80.7	122.4	101.6
	6	99	113.6	134.7	94.3
6	1	91	161.8*	152.6	87.8*
		31/45			

2	77	178.7*	144.1	79.8
3	129	92.2	152.6	95.3
4	111	128.9	115.7	94.1
5	118	66.4	189.4*	98.3
6	99	81.5	134.7	101.2

^{*} Significantly different from control.

The following table summarizes the data for the first five weeks of the study, reflecting the sensitivity of the meiotic and postmeiotic stages of spermatogenesis. Data are represented relative to the control values.

Dose	Relative Lethality (%)	Relative
mg/kg	After Implantation	Survival (%)
150	157.1*	89.0*
30	128.5	100.0
6	157.1*	92.3*

^{*} Significantly different from control.

At these stages, the doses of 6 and 150 mg/kg caused almost the same frequency of dominant lethal mutations. There was no change in the incidence of fertility of the males at the sixth week at any dose level tested.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

14.11.2003 (14)

Type : Drosophila SLRL test
Species : Drosophila melanogaster

Sex : male

Strain : other: Samarkand

Route of admin. : oral feed Exposure period : 2.5-3.0 hours

Doses : 10.5%, 0.75% solutions

Result

Method : other: SLRL test

Year : 1978 GLP : no data Test substance : no data

Remark : (modified test)

Test substance administered to males in 5% glucose feeding

solution; males mated to Oregon K virgin females immediately after feeding treatment. After mating, females were allowed to oviposit immediately or

were held for 6 days prior to ovipositing.

Embryonic lethality was determined by determining the incidence of unhatched eggs after 24 and 48 hours. Post embryonic lethality was determined by scoring the incidence

of larval or pupal death in eggs that had hatched.

Result : Positive. Dose-dependent increase in embryonic lethality;

holding DES-exposed sperm for 6 days prior to oviposition resulted in a marked increase in post-embryonic lethality over controls and non-stored DES-exposed sperm.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

17.12.2003 (16)

Type : other: DNA base sequence changes

Species: Drosophila melanogaster

Sex : male : strain : no data

Route of admin. : oral feed

Exposure period : 3 hours (oral feeding)

Doses : 10, 15, 25 mM (oral feeding), 6.25 mM (injection)

Result :

Method : other: postmeiotic germ cell mutation assay in Drosophila melanogaster

Year : 1993
GLP : no data
Test substance : no data

Remark : oral, injection

Test substance administered to males in buffered 5% sucrose feeding solution or injected in 0.7% NaCl vehicle (0.2 ul). F1 and F2 progeny were screened for occurence of the vermillion (v) mutatation. DNA from 1 g flies was isolated and the vermillion gene amplified using polymerase chain

reaction (PCR).

Result : Base pair substitutions (93%) and deletions (7%) were

induced by treatment with diethyl sulphate; 31

transmissiblevermillion mutants were recovered in F1 and F2 progeny. The most frequent type of alteration were GC -AT

transitions and AT-TA transversions. Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)
UNION CARBIDE CORPORATION Houston

17.09.2003 (23)

5.7 CARCINOGENICITY

Source

Species : mouse Sex : male

Strain : other: C3H/HeJ

Route of admin. : dermal
Exposure period : lifespan
Frequency of treatm. : 3x/week
Post exposure period : none

Doses : 1 brushful per mouse, approximately 7.4 mg/mouse/application

Result : positive

Control group : yes, concurrent vehicle

Method : other: dermal carcinogenicity

Year : 1976 **GLP** : no

Test substance: as prescribed by 1.1 - 1.4

Remark : Three groups of 40 animals each were exposed to the undiluted test

substance, vehicle or positive control substance three times per week via non-occluded application to the clipped back. The animals in the test group were exposed to the undiluted test substance at an average dose of 7.4 mg/mouse/application; animals in the vehicle control group were exposed to acetone at an average dose of 12.6 mg/mouse/application and

the animals in the positive control group were exposed to

methylcholanthrene (as a 0.2% dilution in benzene) at an average dose of 0.033 mg/mouse/application. The test and control substances were applied to each animal with a series 197, number 1 Grumbacher brush. All animals were 8-9 weeks of age at study initiation. Dosing continued until all surviving mice within a group were observed grossly with malignant skin neoplasms or for their lifespan. Dosing was terminated after 22 months in the diethyl sulfate group; after 6 months in the positive control group; and animals in the vehicle control group were dosed for their lifetime.

Result : Repeated dermal application of undiluted diethyl sulphate produced

malignant skin neoplasms in 21 mice out of a

ld 64-67-5 5. Toxicity Date 18.12.2003

surviving effective group of 27 animals. Maximum survival

time for the test group (22 months) was shorter than that of the vehicle control group (27 months); median latent period for appearance of neoplasms was 15.7 months for the test group, 3.7 months for positive control group; no tumors were observed in the vehicle control group.

Source Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

Reliability (1) valid without restriction Flag Critical study for SIDS endpoint

03.11.2003 (34)

Species rat Sex no data Strain other: BD rats Route of admin. gavage Exposure period 81 weeks Frequency of treatm. weekly

Post exposure period

Doses 25, 50 mg/kg

Result

Control group : nο

Method other: Carcinogenicity

Year

GLP no data **Test substance** no data

Remark 12 animals/group; animals approximately 100 days old at

start of treatment: survivors observed until death.

Result Benian papillomas of forestomach observed in 6/24 (number

per group not specified); 2/24 squamous cell carcinoma of

forestomach observed (one per group).

Source Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

12.11.2003

(3)(8)(9)

UNION CARBIDE CORPORATION Houston

Species rat Sex

Strain other: BD rat

Route of admin.

Exposure period day 15 of gestation

Frequency of treatm.

Post exposure period

Doses 85 mg/kg

Result

Control group

Method other: transplacental carcinogenesis

Year

GLP

Test substance no data

Remark Maternal dose = 25% of fetal LD50. Three pregnant females

> injected with test substance on day 15 of gestation; test substance solubilized in an unspecified (probably arachis)

oil. Offspring observed until death.

Result Neurogenic tumors observed in 3 of 30 surviving offspring.

Source Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

12.11.2003 (3)(4)(8)(9)

Species: ratSex: no dataStrain: other: BD rats

Route of admin. : s.c.

Exposure period : 49 weeks

Frequency of treatm. : weekly

Post exposure period

Doses : 25, 50 mg/kg

Result

Control group : no

Method : other: Carcinogenicity

Year

GLP : no data
Test substance : no data

Remark: 12 animals/group; test substance administered as 1.25% or

2.50% solutions in arachis oil. Animals approximately 100 days old at start of treatment; survivors observed until

death.

Result : Local sarcomas observed at site of injection in 11 of

survivors in high dose group with 2 metastases to the lung; there were local tumors in 6/12 rats in the 25 mg/kg group. Historical data indicated that arachis oil did not induce

local timors when injected subcutaneously.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

04.11.2003 (3) (8) (9)

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

Remark: Type: Cohort study.

A historical study examined cancer incidence in 335 process workers who had one or more months employment in an isppropanol plant and an ethanol plant between 1950 and 1976. A total of 225 were still alive, 48 were dead and 32 lost to follow-up. The SIR for laryngeal cancer in this

cohort was 5.04, based on four cases. In an expanded cohort of 740 male workers, the SIR was 3.2 based on seven cases. Interviews of former and present supervisors indicated there were frequent exposures to diethyl sulphate, sulfur dioxide, and ethyl ether. The authors speculate that diethyl sulphate formed during the strong-acid process of ethanol

production, may be the causative agent.

Source : Union Carbide Benelux Antwerpen

ld 64-67-5 5. Toxicity Date 18.12.2003

> ECB - Existing Chemicals Ispra (VA) UNION CARBIDE CORPORATION Houston

23.10.1995 (13)

Remark Type: Cohort study

> A historical control study of the same worker population examined by Lynch found 50 cases of upper respiratory cancer, including 34 larygeal cancers. It was determined that the greatest incidence of upper respiratory tract cancers occurred in workers exposed to high levels of sulphuric acid. Levels of diethyl sulphate were not

measured.

Union Carbide Benelux Antwerpen Source

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (25)

Remark Type: Cohort study

> A mortality study examined the experience of 1031 ethanol and isopropanol production workers from two chemical

plants. Workers were employed for one or more months between 1941 and 1978 were followed through 1983. Among workers exposed to the strong-acid process, there were two deaths from laryngeal cancers (SMR 2.00) and three from cancers of the buccal cavity and pharynx (SMR 1.36); the mortality rate for lung cancers was not elevated (SMR 0.94). No cancer

deaths were seen among weak-acid process workers.

Union Carbide Benelux Antwerpen Source

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (26)

Remark : Type: Case control study.

> Controls without cancer were individually matched to 17 gliomas deaths who had worked at a petrochemical plant between 1955-77. Possible associations between brain cancer and job title, department, history of chemical exposure, location within the plant, dates of employment, and place

ofresidence were examined. Estimated exposure to diethyl sulphate gave an odds ratio of 2.1; duration of exposure

was not related to disease status.

Union Carbide Benelux Antwerpen Source ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995 (12)

Remark : Type: Case control study.

> Controls without cancer were matched to 21 brain cancer cases; 17 were gliomas previously analyzed of using different controls by Leffingwell et al. The proportion of brain cancer cases exposed to diethyl sulphate was

> > (2)

determined to be similar to that of controls.

Union Carbide Benelux Antwerpen Source

ECB - Existing Chemicals Ispra (VA) UNION CARBIDE CORPORATION Houston

23.10.1995

Method

: A Texas petrochemical plant had elevated standardized mortality ratios for neoplasms of the brain. A case-control study examined possible associations between gliomas of the brain and job title, departmental employment history, chemical exposure history, geographic location within plant, dates of employment, and residence. An earlier case control study had also been conducted on the same plant over the

Remark Result : Case-control study of Gliomas of the Brain

No significant differences between cases and controls were apparent in duration of exposure to any of these chemicals, of which many were used simultaneously. The greatest apparent risks were associated with exposure to carbon dioxide, diethyl sulfate, diethylene glycol, ethanol,

ethylene, isopropanol, methane, tetraethylene glycol, and vinyl acetate with first employment in the 1940s or early 1950s, and with residence in La Marque, Texas.

: UNION CARBIDE CORPORATION Houston

16.09.2003 (21)

Method

Source

: Cases consisted of 21 deaths in which the underlying cause was confirmed as a primary brain tumor. Two control groups of 80 employees each were randomly selected from 450 decedents known to the company in June, 1979. Potential exposures while employed were compared between cases and controls for five known or suspect carcinogens. Exposure potentials were also compared for an additional 37 chemicals to which at least four cases were potentially exposed. Overall and 15-year latency analyses were performed.

Remark Result Case-control study of Chemical exposures and Brain tumors45.5% of the employees were exposed to the test substance of

which 40.0% had gliomas. 48.6% and 40.6% were exposed to control 1 and 2, respectively. The proportion of cases exposed to the five potential carcinogenic chemicals were lower than or consistent with the proportion of exposed controls. No statistically significant differences between the proportions of cases and controls exposed to the 37 other chemicals were found. Exposure determinations could not be made for 48% to 57% of the cases and for 56% to 67%

of the controls in each group. This was due to the high proportion of UCC Texas City employees who were assigned to maintenance departments where plantwide travel makes exposure to all chemicals theoretically possible, but

technically unknown.

Source : UNION CARBIDE CORPORATION Houston

27.07.2000 (2)

5.11 ADDITIONAL REMARKS

Type : Metabolism

Remark : Following a single 1 ml subcutaneous, oral, or

intraperitoneal administration of a 5% (v/v) diethyl sulphate solution in arachis oil (59 mg/rat), male rats were housed in metabolism cages and urine collected for 24

hours. Ethylmercapturic acid and a sulfoxide were detected in the urine of DES-treated rats by paper chromatography. The author propose a metabolic pathway involving glutathione

conjugation with one ethyl group.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

16.09.2003 (10)

Type : other: DNA extraction and recovery

Remark : Exposure of HeLa cells in culture to 10 mM DES in 3% DMSO

for 1 hour resulted in a 39.3% recovery of

3Hthymidine-labelled DNA after cold phenol extraction, when

compared to non-treated control cells. Isolated DNA alkylated by DES shows multiple single-strand breaks and denatured DNA. Other techniques were also employed to demonstrate the presence of macromolecular DNA-protein

complexes formed after alkylation with DES.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

23.10.1995

Type : other: Toxicity to fertility

Remark: Diethyl sulphate damaged DNA of E.Coli at the concentration

of 5umol/l.

The substance damages DNA of Hamster ovary at the

concentration of 2.5 mmol/l.

The substance displayed mutagenicity to Hamster gene at the

concentration of 1 mmol/l.

Source : Union Carbide Benelux Antwerpen

ECB - Existing Chemicals Ispra (VA)

UNION CARBIDE CORPORATION Houston

16.09.2003 (17)

6. Analyt. Meth. for Detection and Identification

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- 6.1 ANALYTICAL METHODS
- 6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

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7.1	FUNCTION
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED
7.3	ORGANISMS TO BE PROTECTED
7.4	USER
7.5	RESISTANCE

8. Meas. Nec. to Prot. Man, Animals, Environment

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8.1	METHODS HANDLING AND STORING
8.2	FIRE GUIDANCE
8.3	EMERGENCY MEASURES
8.4	POSSIB. OF RENDERING SUBST. HARMLESS
8.5	WASTE MANAGEMENT
8.6	SIDE-EFFECTS DETECTION
0.0	
8.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
0.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
88	REACTIVITY TOWARDS CONTAINER MATERIAL

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Date 18.12.2003

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10. Summary and Evaluation

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10.1	FND	POIN'	T SU	MMAF	RΥ

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT